SELF-OPTIMIZATION IN SIMULATION-AIDED HIGH POWER MICROWAVE SOURCE DESIGN

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Final Report

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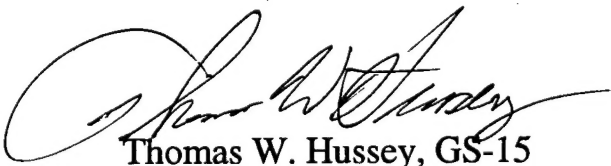This report has been approved for publication.

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14. Abstract
Computer-aided simulation techniques are essential in the design and development of new High Power Microwave sources. Using simulation codes to optimize a process is very slow, however, due to the iterative nature of the optimization, and the true optimal values are never found because the parameters are optimized one at a time instead of the simultaneous minimization process needed for multivariable systems. We have developed a new method that automatically finds the real optimal values by simultaneously minimizing the proper physical quantity versus the relevant variables before the simulation is carried out. There will be no need for repeated execution of nearly identical simulations. The proposed approach will speed up the process at least ten times. A similar approach can be used to speed up non-Particle-In-Cell simulation-aided optimization processes that will benefit the research community in all sectors.

15. Subject Terms
Optimization, Simulation Aided Design, High Power Microwave

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1.0 Introduction

Complex physical systems such as High Power Microwave (HPM) sources attain their peak performance for maximum efficiency only if tuned to optimum values for the relevant parameters. Acquiring the optimal values is straightforward if the system is describable analytically as is the case for very simple systems. HPM sources are far too complex to be described analytically, and alternative means such as numerical simulations are necessary to understand and to optimize them.

Computer-aided simulation is essential in feasibility studies for new concepts, leading to new designs in HPM source development. The Particle-In-Cell (PIC) codes often used to simulate plasma problems and HPM source concepts are very complex in nature, however, and using them to optimize a new source design is particularly labor-intensive and slow. What slows down the process is the inherent need to iterate on the simulation many times before an acceptable design is reached. This process is not only extremely slow, the true optimal values are never found because the parameters are optimized one at a time instead of the simultaneous minimization process needed for multivariable systems. We have developed new mathematical algorithms that automatically find the optimal values by simultaneously minimizing the proper Hamiltonians versus the relevant variables *before* the simulation is carried out. This will find the *real* optimal values all in *one* try. There will be no need for repeated execution of nearly identical simulations to achieve optimization. Considering that the current optimization approach requires as many as a hundred simulations, we believe the proposed approach will speed up the process at least ten times. A similar approach can be used to speed up non-PIC simulation-aided optimization processes that will benefit the research community in all sectors.

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2.0 Interactive Optimization

Numerical analysis afforded by the onset of the digital computer age has revolutionized the way we do research, study new fields, and explore new grounds, scientifically and in practice. Computers can carry out complicated calculations at a faster rate than has ever been humanly possible. This has opened the door to many types of research that was not possible before. Computer-aided numerical methods however, as impressive as they can be by virtue of speed, have their shortcomings compared to pure analytical approaches in basic research. One of these shortcomings is the lack of an easy way for optimization of a physical system evolving under natural forces. It is true that computers can handle large volumes of numerical calculations in a typical simulation problem, but one must not forget that a large portion of those calculations are brought about by the very nature of the brute force computer-aided methods used in simulations. Calculus and variational principle, though powerful optimization tools in mathematics and theoretical Physics are to no avail in computer simulations because of the discrete nature of simulation calculations. Simulations and Monte-Carlo methods are not the most economical ways of finding an optimized system, although they are the only way to find *a* solution to the system, not necessarily optimized. The most elegant way of finding the optimized parameters in a system is through derivatives, and variational principles. Lagrangians used in variational principles are neither available nor useful for complex systems currently solved through simulation and Monte-Carlo techniques. Here, we try to use the concepts behind the variational calculus to speed up the optimization process in simulations.

2.1 The Problem

High power microwave sources, for which this method is developed, are complicated systems involving charge emission, beam transport, rf radiation, rf-plasma interaction, etc. Furthermore, the Physics involved usually dictates a complicated configuration with elaborate geometry and a mix of boundary conditions. The analytical approach, the preferred approach for optimization purposes, is ruled out for all but the uninteresting trivial cases. The analytical approach is ruled out for several reasons. First, the intense nature of the charged particle beams used makes the interactions nonlinear. Few nonlinear theoretical approaches exist dealing with rf-plasma interactions. Second, the complex nature of the boundary conditions makes the algebra too complicated for a manageable analytical approach. Third, and most importantly, the integro-differential equations involved are often so convoluted that no reasonable direct solution can be found. Analytical solution, if possible, come in closed form, containing the answer for every possible parameters and dimensions. This closedness of the solution is what makes it possible to vary the parameters and find the optimal values. This is done through variational methods or by taking the derivative of certain physical quantities.

When there is no analytical solution in closed form possible, we resort to numerical techniques, such as simulation or monte-carlo. These techniques, unfortunately, solve the system for only *one* set of parameters at a time. If one needs to vary any parameter, the entire system needs to be solved again for the new value of that parameter. Since optimization in the normal sense involves a continuous variation of independent parameters in search of maximum (or minimum) dependent variables, optimization through variational methods is not possible for

numerical solutions.

In numerical approach, one starts out a system for a predetermined set of parameters and initial conditions, and follows the evolution of the system for that set of input to any desired length of time. If the set chosen is not the best possible set, as is usually the case, the user has to repeat the process until the best set is found. These simulations will be only slightly different from each other. This "trial and error" approach for finding the optimal set is extremely inefficient and painstakingly slow. For a system with a number of free parameters, every parameter needs to be varied separately, leading to hundreds, perhaps thousands of possible sets. Furthermore, since the parameters can only be varied *one* at a time, the true optimal values can never be found, since that entails a *simultaneous* variation of all parameters. In order to get arbitrarily close to the real optimized values, an iterative method needs to be employed, meaning that the systems needs to be optimized with respect to each parameters several times.

The duration of a simulation of course depends on the problem. A typical high power microwave source simulation problem, even on the fastest computers available in 1997, (tera-flops class), will take one hour. Considering that there is a waiting period of one day in the execution queue for each submittal, we can carry out one simulation a day on mainframe computers. If it takes 100 simulation to optimize a system, a conservative estimate, the optimization will take four months. The process, on a desktop computer, if possible at all, will take even longer. Of course, a more precisely optimized set will require at least one iteration, increasing the optimization time by a factor of two.

The problem then is to find a method to speed up this slow, inefficient optimization process in computer-aided simulation works.

2.2 The Solution

Optimization in simulation aided studies is carried out mostly for one of the three purposes: 1. To maximize the strength of an interaction for the purpose of increasing the growth rate. To this end, we vary the parameters that affect the instability driving the interaction and try to maximize the amount of energy transferred between the interacting bodies. In the case of high power microwave sources, this may be the amount of kinetic energy the charged particle beam loses to the rf fields. The parameters involved are the momentum of the beam, the beam current, the position of the beam, etc. This optimization is important if the mechanism is to be a viable and dynamic means of producing rf radiation. 2. To maximize the efficiency of the operation. Here we try to match the components for the best possible flow of energy from the energizing agent to the desired end product. In the case of rf production, this could mean the proper positioning of the diode, the cavities, the antenna, the proper matching of the load to the device, etc. The overall efficiency is crucial for success of any high power microwave source. 3. To configure the best possible layout for the size and the geometrical design of the device. In the case of high power microwave production this means the best dimensions for the oscillator cavities, the waveguides, the diode, etc. This optimization is important in the usefulness and the overall efficiency of the device. In each of the three cases described here, there is always a "physical quantity" that

contains the relevant parameters controlling that aspect of the operation. This quantity, if identified and chosen properly, can be easily calculated and used in the subsequent operations.

The basic structure of an interaction or the basic layout of a new device is normally determined in the conception phase of the effort. When possible, analytical studies can further refine the structure providing a framework for the starting configuration in a simulation. However, because of the qualitative nature of the conceptual data and the analytical results lacking the sophistication of the real situation, simulations often fails to produce the best results in the first few attempts. Conventional numerical methods such as simulation do not search for optimized input parameters. Optimized input parameters need to be found before a simulation can produce optimized results.

The work presented here introduces a method for finding the optimized input parameters interactively as the simulation is being carried out. We propose to produce a Particle-In-Cell (PIC) simulation code that *optimizes* the data it uses for the simulation. The approach will be to start out with the approximate input data that the user provides and simultaneously maximize a *performance indicators* (growth rate, efficiency, geometry, etc.) with respect to the parameters the user deems essential. The optimization will be done by forming the proper "performance indicator" numerically, taking the derivatives with respect to the relevant parameters numerically, and solving for the optimized values. The solution will be best obtained using an iterative process that suits the finite difference nature of the PIC algorithms. The overhead associated with this initial optimization will be insignificant compared to the simulation CPU usage because the optimization will only be done once at the beginning of the simulation run.

2.3 The Approach

Based on the nature of the optimization needs, a performance indicator is first identified. The performance indicator is a physical quantity closely associated with the physical aspect being optimized. For instance for optimization of an "interaction", the Hamiltonian or the Lagrangian would make good performance indicators. To optimize the growth rate, the net energy transferred from the beam to the rf fields is a good performance indicator. The saturation amplitude is a good indicator of the overall efficiency. The performance indicators are functions of a large number of parameters whose numerical values need to be known at the time of the optimization. The choice of the performance indicator and the parameters it depends on are very important in the success of this approach. We need to pick a performance indicator that contains at least one *sensitive* parameter in the optimization. An experienced simulation analyst will have no problem identifying a suitable performance indicator for the case at hand.

Once a performance indicator is identified and its form determined, a brief search, either analytically if possible or numrically, will be conducted to find the most sensitive parameters to vary. The choice for the sensitive parameters is often trivial based on the user's knowledge of the device. The next step is to start a simulation run based on the user's provided set of best guess inputs. The best guess values come from crude analytical estimates or from prior knowledge of the device. The simulation starts like a normal run, advancing the system evolution in time far enough to have meaningful numerical values for all physical quantities calculated, and in

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particular for the performance indicator picked for the case under study. At this point the normal execution is interrupted and the following procedure is carried out.

The numerical value of the performance indicator is optimized by simultaneously varying the relevant parameters. This is the numerical equivalent of solving a set of n equation, n unknowns,

$$\delta(p_1, p_2, \ldots p_n)/\delta p_i \quad i=1,n$$

This will require advancing the simulation by another time step or two in order to calculate the performance indicator for the varied parameters. Also remember that numerical optimization of a set of equations is an iterative process that might require a number of iteration until the maxima or the minima of the performance indicator are found. Any number of iterative techniques may be used. The Newton-Raphson method was used in our approach. To find the true optimized values, care must be taken to make sure all the maxima and minima are found, not just the local ones.

The resulting set $(p^o_1, p^o_2, \ldots p^o_n)$ is the desired set of parameters that optimize the device or the interaction. In practice, there is usually only a small number of parameters (two or three) that are sensitive enough to be optimized for any category. Some interesting cases can be optimized with only one parameter to vary.

The code chosen for this optimization enhancement was the three-dimensional parallel PIC code ICEPIC currently being developed at the Phillips Laboratory for use on massively parallel computers.

The optimization algorithm chosen is a Fibonacci (or Golden Section) search. It can be shown that this algorithm is optimal when only discrete function samples are taken. The optimization algorithm was implemented in ANSI C for portability and tested on a number of analytic functions. It has proved satisfactory to a user-defined fractional tolerance limited only by machine precision. A simple parser was written to filter input decks for the optimizer. This code, along with the code necessary to spawn the separate ICEPIC jobs was incorporated with the optimizer. A measure of microwave output has been successively refined to provide a more accurate metric for optimization.

3.0 Test-case Results

To validate the effectiveness of the method in finding the optimized set of parameters in a real HPM source, we applied the method to an already well optimized source and compared the results with previously known values. The test-case chosen was an HPM source called Transvertron. The transvertron is a multi-gigawatt rf oscillator designed for efficiency and high power. It is a transit-time oscillator converting the kinetic energy of an Intense Relativistic Electron Beam (IREB) into a monochromatic intense rf radiation in the L-band. There is no need for an external magnetic field.

The transvertron consists of a conducting cylindrical cavity, approximately 15 cm long, 31 cm in diameter, crossed by an annular beam of electrons travelling axially near the outer wall. The beam thickness is 6 cm, the beam current is 30 ka and the kinetic energy of the beam is 3 MV. The parameters involved are the dimensions of the cavity, namely the length L, the radius R, the beam electrical parameters the current I and the voltage V, the beam thickness D, the beam location P, the external magnetic field B, and the cavity quality factor Q. Other parameters such as temperature, residual magnetic fields, beam divergence, etc. are not sensitive enough to play an important role in the operation of the device.

The Physics of the transvertron is simple. When the transit time of the beam particles matches the period of one of the characteristic modes of the cavity, the electrons will be facing a decelerating electric field more often than an accelerating one, so that the beam on the average looses kinetic energy to the rf fields. This constitutes the mechanism for the growth of rf radiation in transvertron, and in all transit-time oscillators in general. Saturation is reached when the rf fields are large enough to modify the transit-time of the beam particles, destroying the resonant condition for the growth.

Figure 1 is a schematic drawing of the device shown with the beam particles trajectories after saturation, as modeled by the simulation code MAGIC. Only the upper half is modeled. The trajectories show the paths of the particles for one time step. The stray particles near the axis are particles reflected by the rf fields, indicating that the rf fields have exceeded the dc field values, typical of unloaded transit-time oscillators. Matched loading will lower the rf amplitudes to below wave breaking levels.
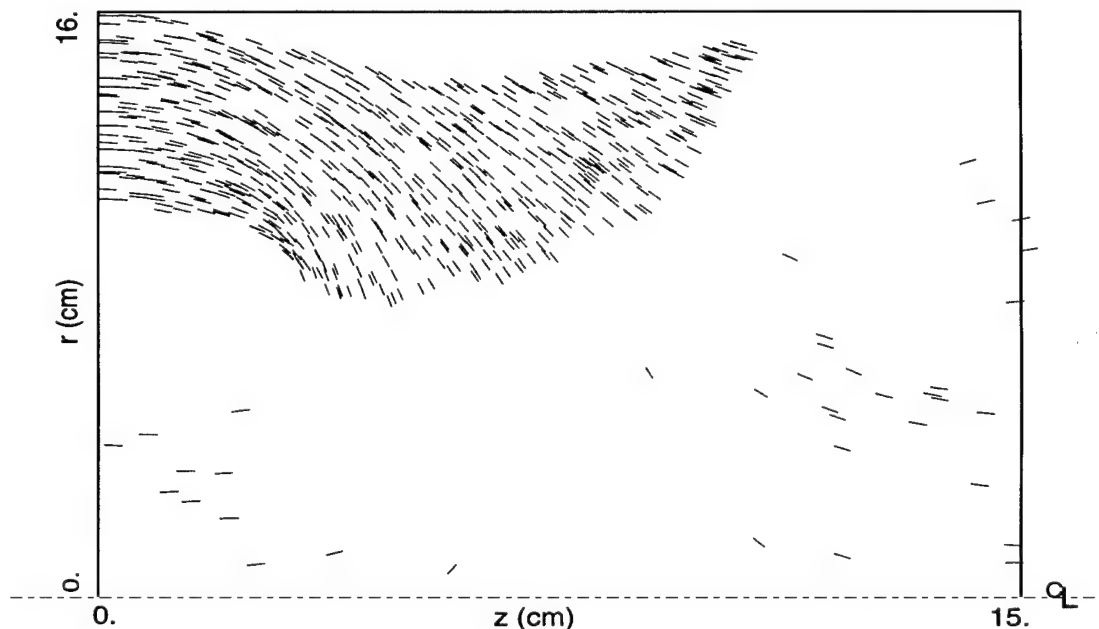

Figure 1. Axial section of the Transvertron shown with the beam after saturation.
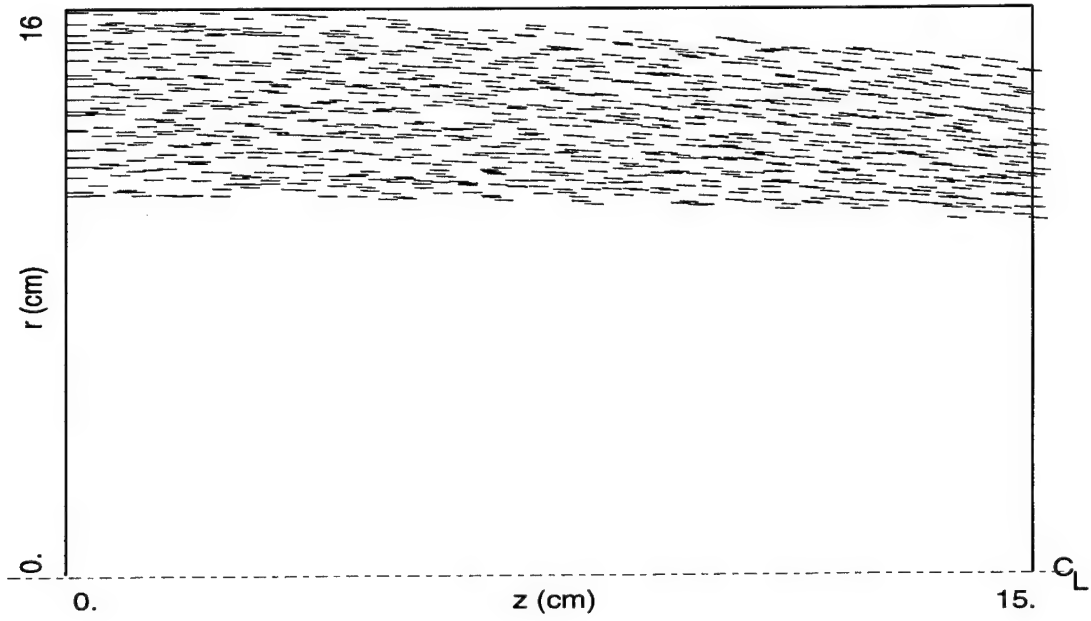The device shown here is optimized for maximum efficiency

Figure 2. Axial section of the Transvertron shown with the beam before saturation,
at the time of optimization.

As a first trial, the length of the cavity was selected as the varying parameter, and varied interactively to find the fastest growth rate, keeping other parameters fixed. The length is one of the two most sensitive parameters for this device. The other sensitive parameter is the beam kinetic energy, which is not strongly coupled to the length, and may be varied independently without modifying the optimization with respect to the length. The performance indicator chosen was the "kinetic energy transferred" from the beam to the rf fields over one oscillation period. This device oscillates at 1.3 GHz, the frequency for the TM_{011} mode for a cylindrical cavity at these dimensions. The performance indicator was formed by adding the kinetic energy of the beam particles in the cavity and averaging it over one period T, namely 0.76923 ns. Since the optimization was carried out versus the cavity length, the performance indicator was normalized to the unit length to eliminate the increase of the kinetic energy due to the length. The optimization was of course carried out a long time before the onset of saturation.

Figure 2 is a plot of the beam trajectories at the time of optimization, 15 ns into the simulation. The time to saturation is 50 ns. The optimization may be carried out even sooner depending on the beam risetime. The risetime chosen here is 5 ns to cover approximately 6 oscillation periods. Any risetime shorter than 5 ns might excite transient modes that will complicate the optimization process.

The optimization scheme implemented in the code ICEPIC was instructed to start out with a low value for the length, namely l=13 cm, and proceed to find the best value for maximum growth rate. Figure 3 is the time plot of the radial potential at the center of the L=13 cm cavity. This potential is a good indicator of the TM_{011} mode growth in the cavity. The voltage integration was

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carried out at the center of the cavity because that is where the radial electric field component E_r is the maximum. Of course, the larger the growth rate, the faster the rf fields will grow and saturate. The slight offset in the zero-crossing for the potential is due to the coarseness of the cells in the simulation and the difficulty associated with choosing the potential exactly at the center. For this simulation with L=13 cm, the potential amplitude is still on the rise after 50 ns. This same run, when continued to 80 ns, Figure 4, saturated at approximately 73 ns. Figure 5 is the same time plot but for the optimum length cavity, L=15 cm. The growth rate is much faster and the saturation is reached after approximately 47.5 ns. This optimum value for the length was reached using the interactive optimization technique described above. The optimized value of l=15 cm agrees very well with the previously known values obtained through conventional methods. The ratio of the saturated amplitude of 7.5 MV in figure 4 to the input voltage of 3 MV is also a good indication that l=15 cm is a good optimized value for the length of the cavity. Of course, how close we will get to the exact value for the optimum length, will depend on the size of the cells chosen. The finer the cell sizes, the more exact the optimum value will be. The cell size chosen here was 0.5 cm. This means the exact optimum value will lie between 14.75 cm and 15.25 cm. Figure 6 is an overlay of the voltages for the starting value of l=13 cm for the length and the optimized value of l=15 cm, plotted on the same time scale. The optimized case grows much faster than the trial case.

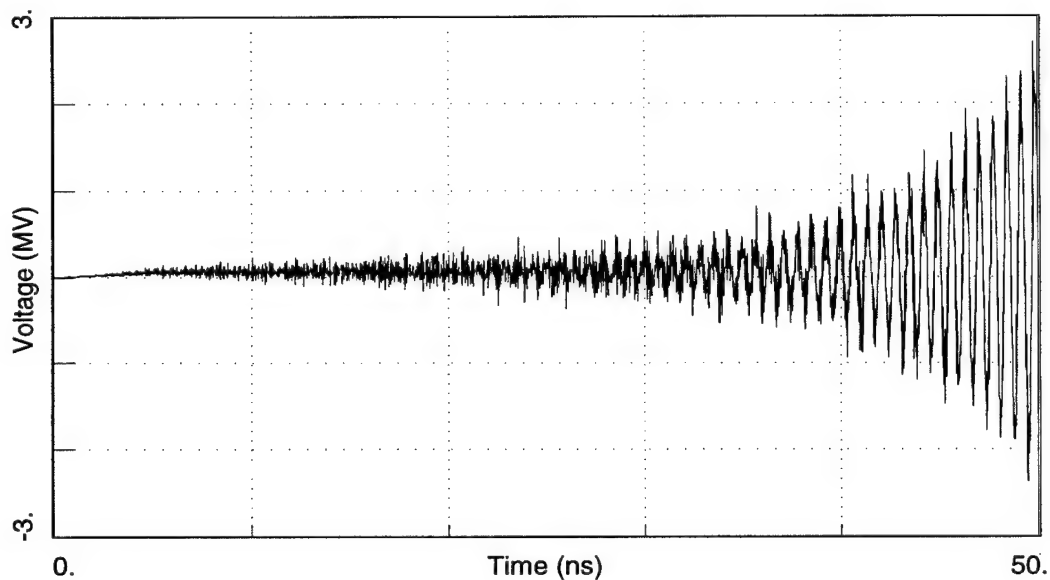

Figure 3. Time plot of the radial voltage at the center of the L=13 cm cavity.

The saturation is not reached after 50 ns.

The search took a total of 4 tries to zero in on the optimum value for the length. A total of ten simulations were carried out to complete the optimization curve. Of course, tracing out the complete optimization curve is not necessary for finding the optimum values, it was carried out for comparison purposes. In fact, the optimization runs need not be carried out to saturation. The four runs carried out for optimization, were continued to only 15 ns.

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It should be emphasized that the nature of this optimization approach is very general. It will work on any device, any interaction, or any instability, for any set of parameters. The transvertron was chosen here as a test-case because of its simplicity, and the level of independence among the parameters involved. A clear comprehensible comparison with a well established, otherwise optimized case, such as transvertron, is essential in demonstrating the viability and effectiveness of this new approach.
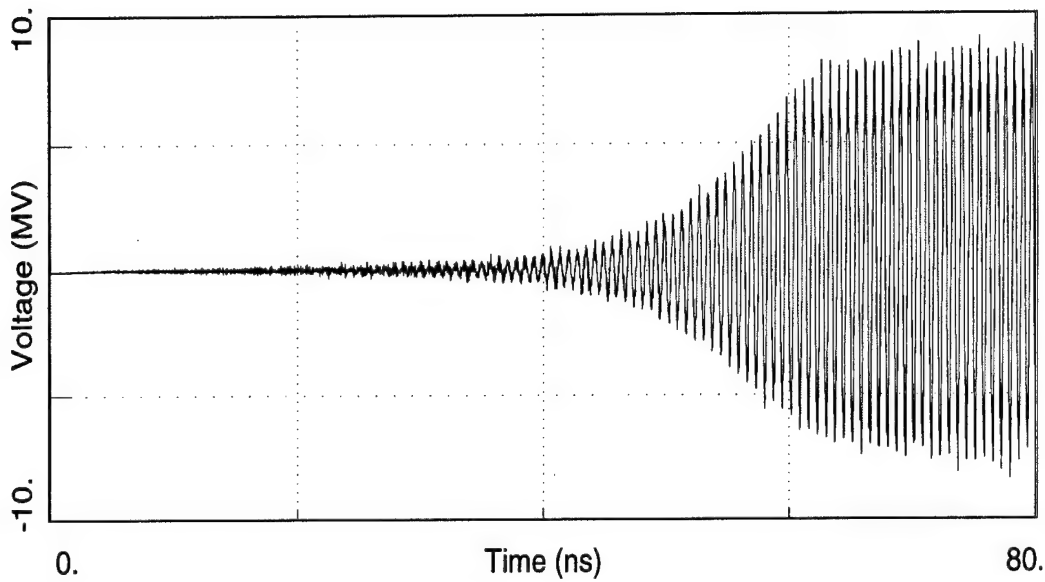

Figure 4. Time plot of the radial voltage at the center of the non-optimized case. Time to saturation is approximately 73 ns.

Some performance indicators, such as saturation amplitude, are hard to optimize because the corresponding physical quantity does not have a closed form. In such cases, one either establishes a link between the desired quantity and an optimizable quantity, or uses conventional methods to optimize. For instance, to optimize the efficiency in the transvertron, the beam-cavity coupling is a good performance indicator to optimize because the efficiency is strongly linked to this coupling.

Finding the sensitive parameters the in optimization processes is an important step. This may be done analytically, if the process or the device can be simplified to an analytically manageable form. In more complex cases, the new method introduced here may be used to find the desired parameters. The process consists of forming the performance indicator in its most complete form including as many parameters as possible and numerically taking the derivative with respect to every parameter to find the steepest slope. This process must of course be carried out prior to the optimization process in order to select a suitable set of parameters to include in the optimization. If many parameters turn out to be sensitive, then the parameter finding process becomes part of the optimization itself.
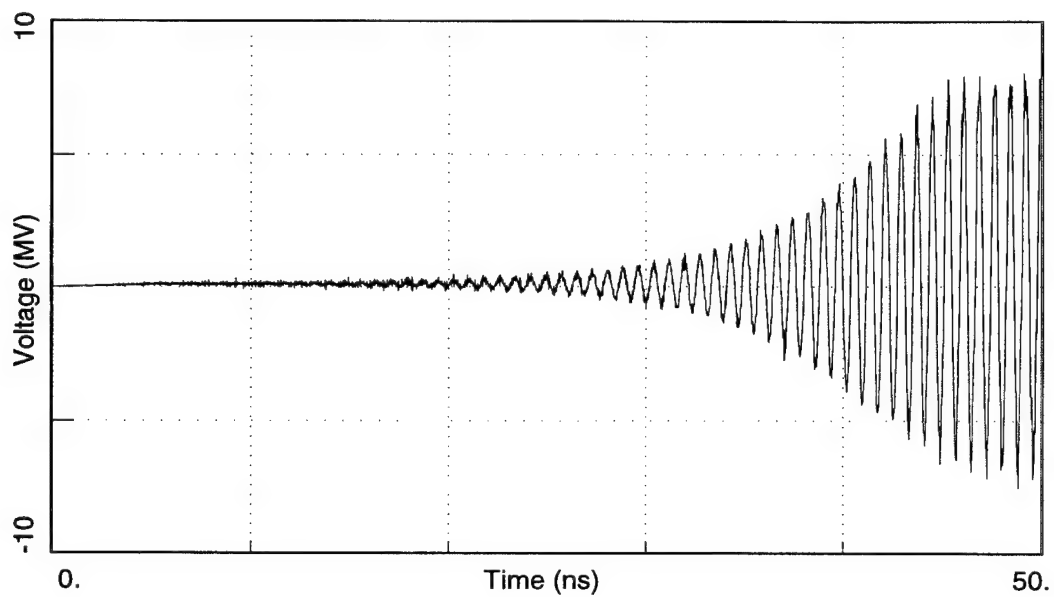
Figure 5. Time plot of radial voltage at the center of the optimized cavity.
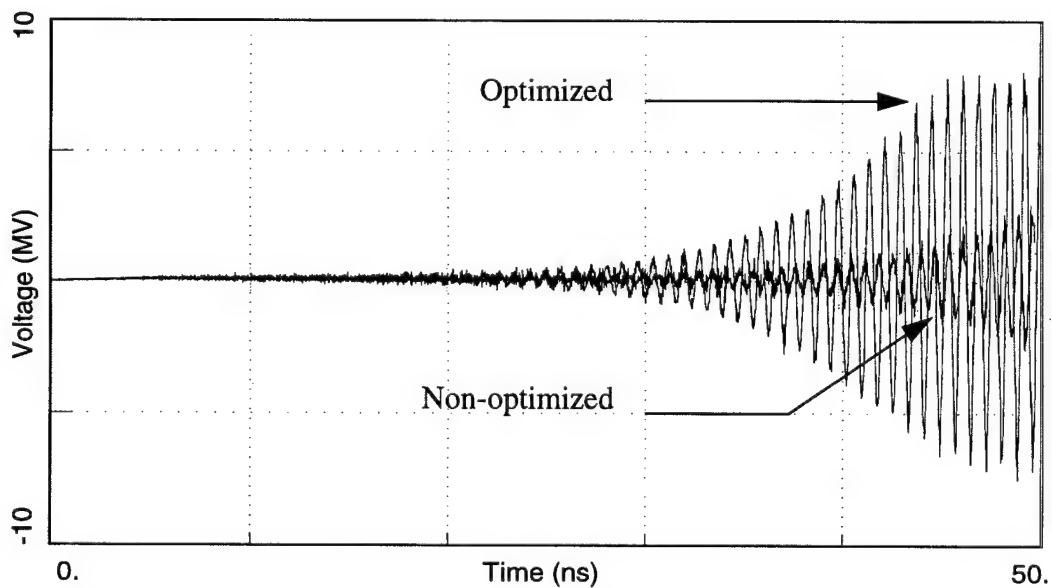The saturation is reached after approximately 4.75 ns.

Figure 6. Overlay of the radial potentials at the center for the L=13 cm
and the optimized cavities. The optimized case grows faster.

Figure 7 is the optimization curve with respect to the length of the cavity. It was constructed by running the simulation for a number of points near the optimum value to verify that the optimum value indeed gives the best growth rate possible in that region. There is of course no need to construct this curve with every optimization. It was carried out here to show the validity of the new approach presented. Constructing this curve is indeed equivalent to the conventional way of finding the optimum value. We also used this curve as a basis for finding the speed up associated with the new method. The speedup of course varies from case to case, and the larger the number of interrelated parameters to optimize, the larger the speedup factor will be. For the simple case considered here with only one variable involved, the speedup will be modest. The new method zeroed in on the optimized value of L=15 cm 11 times faster than the old method of constructing the optimization curve. We anticipate that the speedup factor will be proportional to $n^{1/2}$, the square root of the of number n of the dependent parameter optimized. i.e., for an optimization with 4 parameters, the speedup will be a factor of 22 for this case.
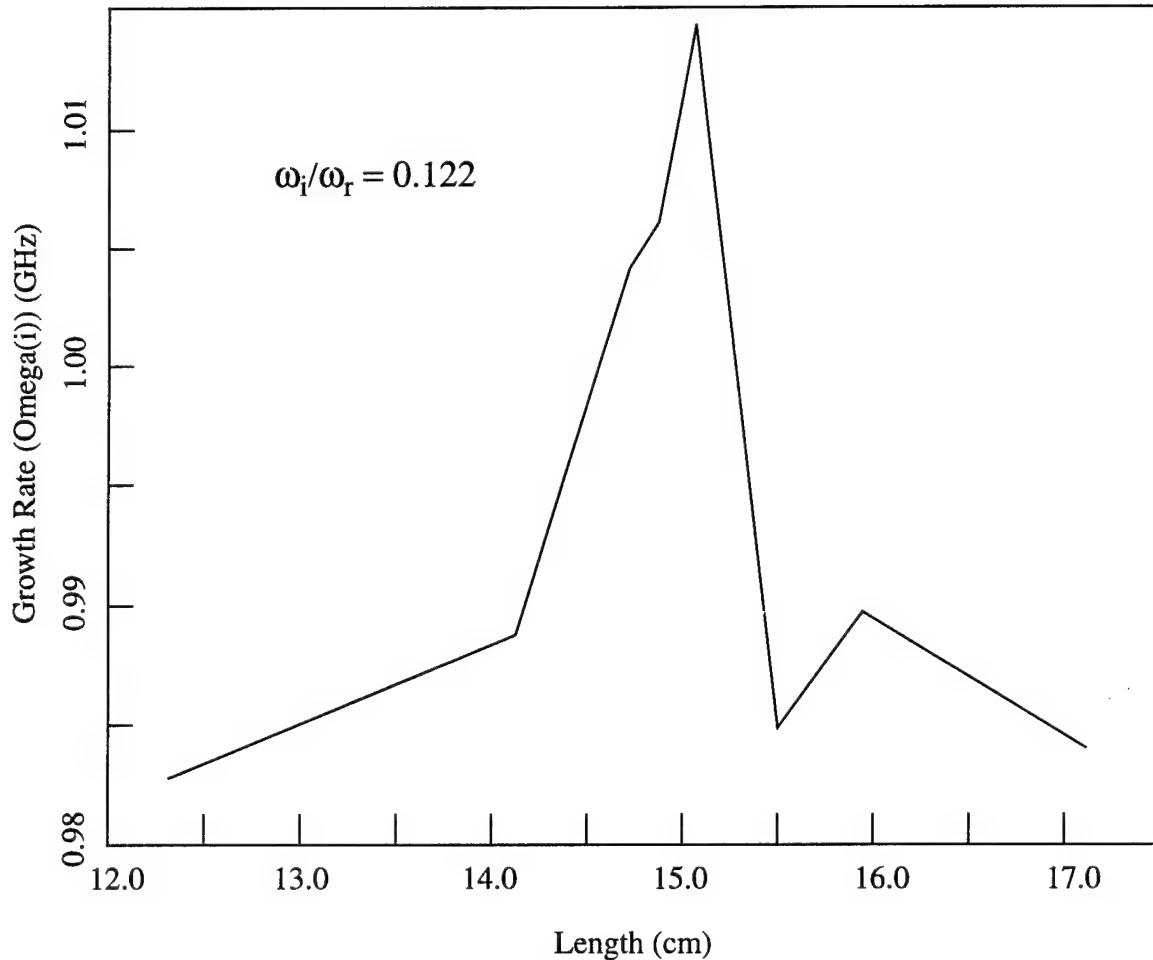

Figure 7. The optimization curve for the growth rate as a function of the cavity length. The growth rate peaks at L=15 cm.

The kinetic energy of the beam for the Transvertron is also a sensitive parameter in the optimization of the growth rate. Figure 8 is the optimization curve for a conveniently chosen performance indicator tied to the efficiency, plotted versus γv, where γ is the relativistic factor for the beam and v is the velocity of the beam. γv is in fact the electron beam momentum divided by the electron mass. This optimization was also carried out as a single parameter search, with all the other parameters fixed. The optimized value of the cavity length was used in this optimization. Since a near-optimized value for the beam momentum was used in the length optimization, no significant increase in the growth rate was observed as a result of this optimization. The optimum value for the beam kinetic energy was found after five tries. A total of 21 simulations were carried out to construct the optimization curve in Figure 8. The optimization was carried out to verify the validity of the new optimization method. The speedup factor observed was 10.4.
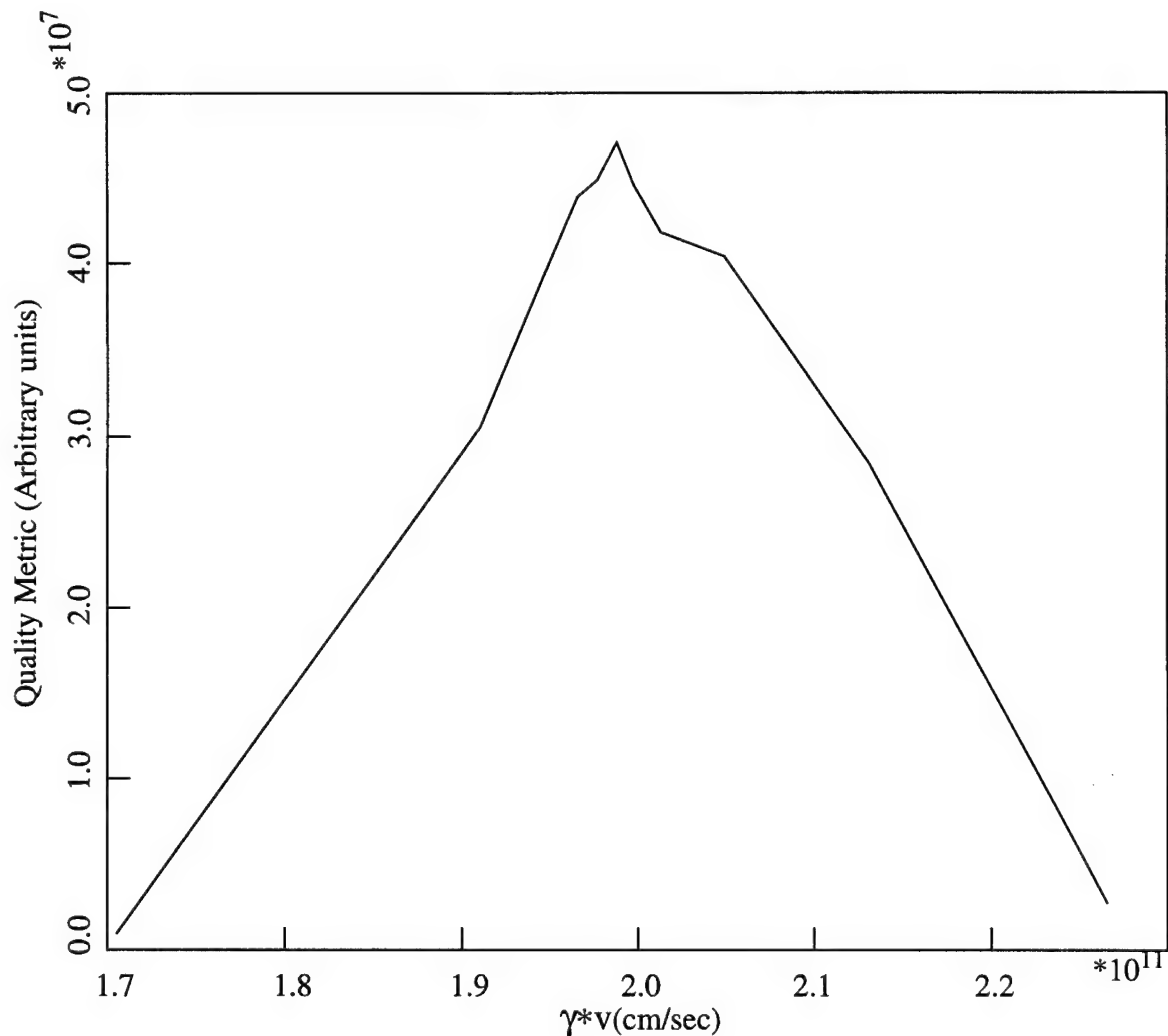

Figure 8. The optimization curve for the Transvertron efficiency as a function of the beam momentum.

4.0 Conclusions

We have demonstrated that the optimization method developed here can speed up the conventional numerical optimization process by at least a factor of ten. The speed up is higher for more complex systems, involving a large number of parameters. The method is modular, efficient and relatively easy to implement. It can be easily integrated into any existing simulation code, and may be modified for each case separately. It may also be formulated in a comprehensive way to make it general for either single or multi-parameter optimization. Further generalization to allow multiple performance indicators is not much harder.

Efforts have already begun that will give the optimizer greater power and a user friendly interface. A more sophisticated parser has been written that will allow the user to make definitions in the template input deck and perform algebraic operation on these defined variables and the varying parameters of the optimization within the input deck. These improvements will be necessary if the optimizer is to be run on more complicated device simulations without "hard-wiring" knowledge of these devices into the simple parser currently in place in the optimizer. Also, these first improvements are necessary to extend the optimization search beyond functions of a single variable to functions of multiple variables.

The algorithms for the optimization of a function of multiple variables have been identified for possible use in a future versions of the optimizer. This will allow simultaneous optimization with respect to a number of variables for greater accuracy and further speedup.

The approach developed here is, of course, not limited to PIC simulation, or even plasma simulation methods. The concepts introduced may be used in any simulation in any field or discipline. The method can still be used even if no performance indicator in a closed form can be found for a particular parameter. Because of the redundancy usually present in formulating the chosen performance indicators, a parameter closely tied to the desired parameter may be optimized with similar effects.

The numerical analyses based on Monte Carlo techniques can also be enhanced using this approach. All the necessary data and data structures for the optimization are already available in a Monte Carlo calculation. The optimization can be carried out prior to the normal monte Carlo calculation for an optimized calculation.

Publication

The following article is being prepared for submission to the *IEEE Transactions on Plasma Sciences* for publication

Interactive Optimization, a Numerical Approach to Fast Simulation-Aided Microwave Source Design

Presentation

The following topic was presentation at the 1996 meeting of the APS Division of Plasma Physics, Denver, CO. The optimization method presented here was used to optimize this device.

Loading of Phase-Locked Radial Klystron Oscillator.

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